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Sensitivity analysis of temporal parameters in a dynamic LCA framework

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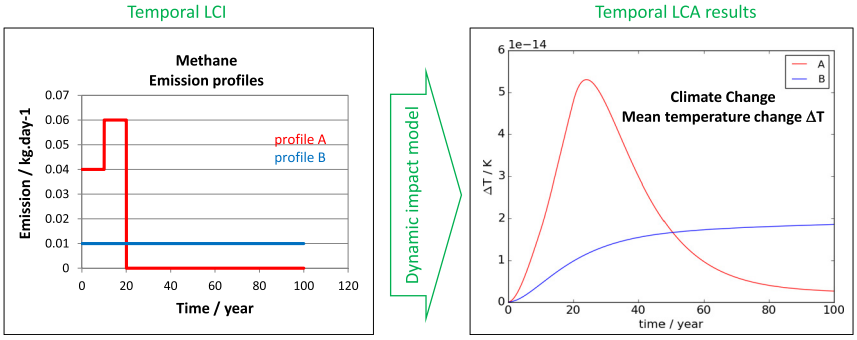
HIGHLIGHTS

- Dynamic LCA framework interconnects temporal inventory and dynamic impact models.
- Dynamic climate change is not sensitive to LCI time steps lower than 1 year.
- Dynamic (eco)toxicity indicators are very sensitive to LCI temporal definition.
- A predefined time horizon has no interest and relevance for dynamic LCA models.

GRAPHICAL ABSTRACT



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ABSTRACT

Including the temporal dimension in the Life Cycle Assessment (LCA) method is a very recent research subject. A complete framework including dynamic Life Cycle Inventory (LCI) and dynamic Life Cycle Impact Assessment (LCIA) was proposed with the possibility to calculate temporal deployment of climate change and ecotoxicity/toxicity indicators. However, the influence of different temporal parameters involved in the new dynamic method was not still evaluated. In the new framework, LCI and LCIA results are obtained as discrete values in function of time (vectors and matrices). The objective of this study is to evaluate the influence of the temporal profile of the dynamic LCI and calculation time span (or time horizon in conventional LCA) on the final LCA results. Additionally, the influence of the time step used for the impact dynamic model resolution was analysed. The range of variation of the different time steps was from 0.5 day to 1 year. The graphical representation of the dynamic LCA results shown important features such as the period in time and the intensity of the worst or relevant impact values. The use of a fixed time horizon as in conventional LCA does not allow the proper consideration of essential information especially for time periods encompassing the life time of the studied system. Regarding the different time step sizes used for the dynamic LCI definition, they did not have important influence on the dynamic climate change results. At the contrary, the dynamic ecotoxicity and human toxicity impacts were strongly affected by this parameter. Similarly, the time step for impact dynamic model resolution had no influence on climate change calculation (step size up to 1 year was supported), while the toxicity model resolution requires adaptive time step definition with maximum size of 0.5 day.

1. Introduction

Life Cycle Assessment (LCA) is a widely used methodology for evaluating products and processes. LCA methodology consists of four

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operational steps: the definition of the goal and scope, the construction of the Life Cycle Inventory (LCI) based on mass and energy balances over the whole life cycle of the system, the Life Cycle Impact Assessment (LCIA) based on various impact calculation models, and the interpretation step (ISO, 2006a; ISO, 2006b). One of the recognized limitations of the LCA method is the lack of a time dimension in the definition of both the LCI and LCIA steps (Finnveden et al., 2009). Such a time dimension has only recently been integrated into LCA and little research is currently in progress.

Beloin-Saint-Pierre et al. (2014) have developed an approach called Enhanced Structure Path Analysis for considering time in the LCI step. Cherubini et al. (2011) have performed a calculation considering dynamic carbon removal by the biomass, which is a step leading up to the calculation of the climate change impact, while Levasseur et al. (2010) and Kendall (2012) have studied the time dependency of climate change impact by calculating temporal characterization factors (CF) for substances and applying them to dynamic emissions. Huijbregts et al. (2000a, 2000b, 2001), Hellweg et al. (2003) and Lebailly et al. (2014) have also proposed adjustments of conventional methods to include temporal characteristics in the toxicity category. In a recent study, Beloin-Saint-Pierre et al. (2017) proposed a complete framework for the calculation of a dynamic LCA. Tiruta-Barna et al. (2016) provided a dynamic method for LCI in which they took the complex supply chain and processes present in the LCA system into account. Their method can be linked to a conventional LCA database, which facilitates its use by LCA practitioners. Shimako et al. (2016, 2017) applied this dynamic LCI method in two different case studies, combining it with a dynamic climate change model and a dynamic toxicity model.

Numerous parameters can influence the temporal profile of a dynamic LCA result. At LCI level, these are physical parameters describing the process and supply chain dynamics, the time scale and its granulometry, and also specific parameters of the numerical methods used for model resolution. Dynamic LCIA results are determined by the choice of the impact models/submodels (i.e. static or dynamic) and their physical parameters, along with numerical method parameters.

The processes and phenomena involved in all these models are characterized by very different dynamics and thus prioritization of the most influent parameters is a necessity in the development of a dynamic LCA method.

Dyckhoff and Kasah (2014) analysed the influence of a time horizon in the calculation of the dynamic global warming potential indicator. A comparison between the cumulative and instantaneous indicators demonstrated that contradictory conclusions could be drawn when different time horizons were used in calculations. The choice of a time horizon depends on the decision maker and is based more on policy than on scientific considerations. To the best of our knowledge, other important temporal parameters have not been analysed yet.

Sensitivity analysis is a valuable tool to evaluate the contribution of the temporal inputs to the dynamic results. There is general agreement that the input parameters of a model are sensitive in two distinct manners: (1) the uncertainty associated with an input parameter which is propagated in the model and contributes to the uncertainty of final results, or (2) the strong correlation between the inputs and outputs, such that a small change in the input leads to large changes in the output (Hamby, 1994). It is the second aspect that, at this stage of development of the dynamic approaches in LCA, allows the importance of the temporal parameters' influence on the LCA results to be identified, and will finally help further developments.

The objective of this work is to study the influence of temporal parameters involved in the dynamic LCA methodology we are currently developing. The global dynamic LCA framework was developed by using the dynamic inventory method proposed by Tiruta-Barna et al. (2016) and the dynamic impact assessment proposed by Shimako et al. (2016) and Shimako et al. (2017). One of the primary questions is how the dynamic LCI profile and the details of the inventory temporal definition will influence the final LCA results. In the aim of answering this question, a sensitivity analysis was conducted on a case study: a waste water treatment plant life cycle. The choice of the case was guided by the high temporal variability of the physical parameters involved in the process, leading to a complex LCI temporal profile.

2. Methods

2.1. Dynamic LCA framework

2.1.1. Global framework

The global framework for dynamic LCA is presented in Fig. 1.

First, SimaPro® LCA software was used for the traditional LCI resolution. This software delivers the LCI results in matrix form: a technological matrix and an environmental intervention matrix (interventions by compartments and processes). The dynamic inventory model and the DyPLCA software (web application http://dyplca.univ-lehavre.fr/) start from the conventional inventory matrix to create the process flow network as a graph structure and then adds temporal parameters related to processes and supply chains. After computation of the inventory model on the graph structure as a function of time, this tool delivers a time vector (days) and the associated environmental intervention vector (specific units·day^{-1}, e.g. kg·day^{-1}). Besides the temporal parameters specific to the processes and supply chains, the computation of a dynamic inventory requires specific parameters for the numerical methods (Fig. 1): time step size of graph resolution and consequently the time step size with which the LCI is calculated (e.g. values of inventory at each 0.5 day), backward time limit (the algorithm will stop when reaching a specific value of time backwards), numerical precision of the results and threshold (lower limit of the mass flow value that the algorithm will consider).

The result of the dynamic inventory, i.e. environmental interventions distributed in time, is used for the calculation of dynamic climate change and toxicity impact categories. Homemade Python programs were developed with this aim. For the calculation of dynamic impacts, data and phenomenological dynamic models were implemented: (i) from IPCC (IPCC, 2013) for climate change, and (ii) from the USEtox® 2 model (Hauschild et al., 2008; Rosenbaum et al., 2008) for toxicity categories.

The parameters required for both climate change and toxicity, in addition to specific phenomenological parameters, are the time span for the impacts calculation and the time step size for the numerical calculation and for results retrieval. The maximum step for the ordinary differential equations (ODE) solver used to find the mass balance in the toxicity dynamic model must also be specified.

The principles of the dynamic models for climate change and toxicity impacts are briefly described below.

2.1.2. Dynamic climate change model

The dynamic climate change impact category was evaluated through two indicators: radiative forcing and global mean temperature change. The atmospheric burden, B_s, is an important parameter in the modelling of climate change potential. It can be calculated as the convolution product between the dynamic emission of the substance s, g_s (kg·day^{-1}) and the impulse response function of that substance, IRF_s (Olivié and Peters, 2013):

$$B_s(t) = \int_0^t g_s(t')\, IRF_s(t-t')dt' \quad (1)$$

where t and t' are time scales. Radiative forcing is described as the product between the radiative efficiency, A_s, and the atmospheric burden, B_s. For sufficiently small emissions and approximately constant background conditions, the radiative efficiency A_s (W·m^{-2}·kg^{-1}) can be approximated as time-invariant (Joos et al., 2013). For emissions starting

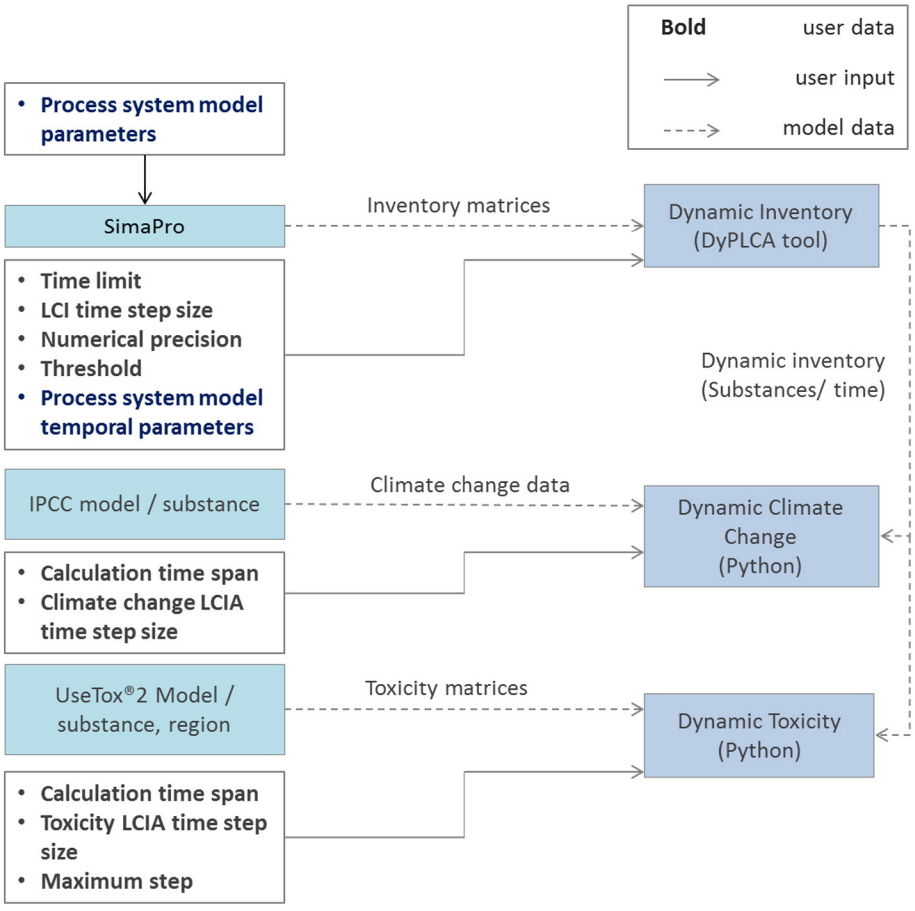

Fig. 1. – Parameters needed for the dynamic life cycle model in LCI and LCIA steps.

at time t_0 we have:

$$n_{\text{radiative forcing,s}}(t) = \int_{t_0}^{t} A_s(t) g_s(t') IRF_s(t-t') dt' \quad (2)$$

The dynamic global warming potential ($n_{\text{radiative forcing}}(t)$ in $W \cdot m^{-2}$) for all gases taken together is then:

$$n_{\text{radiative forcing}}(t) = \sum_s n_{\text{radiative forcing,s}}(t) \quad (3)$$

Then, the global warming potential for all gases ($n_{\text{radiative forcing}}$ in $W \cdot m^{-2} \cdot day$) over a given time span TH is:

$$n_{\text{radiative forcing}} = \int_{t=t_0}^{TH} n_{\text{radiative forcing}}(t) dt \quad (4)$$

The second indicator, i.e. global temperature potential, is defined as the convolution product between the radiative forcing and the temperature impulse response function (Olivié and Peters, 2013):

$$n_{\text{temperature,s}}(t) = \int_{t_0}^{t} \left(\int_{t_0}^{t} A_s(t) g_s(t') IRF_s(t-t') dt' \right) IRF_T(t-t') dt' \quad (5)$$

where $n_{\text{temperature,s}(t)}$ is the global temperature potential for a substance s at time t and IRF_T is the temperature impulse response function, which is independent of the type of GHG. The mean temperature change at a given time t, $n_{\text{temperature}}(t)$ (K), is obtained by aggregating values for all the substances concerned:

$$n_{\text{temperature}}(t) = \sum_s n_{\text{temperature,s}}(t) \quad (6)$$

2.1.3. Dynamic toxicity model

The dynamic toxicity approach was developed in Shimako et al. (2017) and only a brief background is presented below. Traditionally, toxicity impact is calculated as the product of the substance mass and its characterization factor (CF). CF is the result of combined models for substance fate in environment (fate factor), exposure of organisms to the hazardous substance (exposure factor) and the negative effects of the substance (effect factor). The dynamic approach replaces the fate factor by a dynamic model of substance fate while keeping the exposure and effect factors from the conventional approach. The fate model of a substance in the environment considers distinct mechanisms, such as the transport between compartments, reaction processes (e.g. degradation), and removal (immobilization in different media). The mass balance of a substance in the environment is described by a system of ODE (Mackay, 2002):

$$\frac{dm_s}{dt} = K_s m_s + g_s \quad (7)$$

where K is the square matrix of rate constants (related to removal, degradation and transport processes) in each compartment i (day^{-1}), m is the mass vector of substance s in the respective environmental compartments (kg), g is the vector of emission flows in each compartment ($kg \cdot day^{-1}$), and t is time.

The generic dynamic fate model was adapted with the USEtox toxicity model (specific parameters per substance and phenomenon, 13 environmental compartments; Jolliet et al., 2006; Ligthart et al., 2004; McKone et al., 2006). By the end of the calculation, a mass vector (13 values corresponding to each compartment) had been obtained for each discrete time value. For the toxicity results, following the matrix approach proposed by Rosenbaum et al. (2007), each mass vector is multiplied by the exposure matrix (*XF*) and effect matrix (*EF*):

$$n_{human,s}(t) = m_s(t) \times XF_{human,s} \times EF_{human,s} \quad (8)$$

$n_{human,s}(t)$ is the vector that represents human toxicity (cancer and non-cancer, cases·day^{-1}) for a certain substance s in different compartments, at a given time t.

$$n_{eco,s}(t) = m_s(t) \times XF_{eco,s} \times EF_{human,s} \quad (9)$$

$n_{eco,s}(t)$ represents the ecotoxicity expressed in (PAF·m^3·day)·day^{-1}, due to an emission into a specific compartment for a certain substance s at a given time *t*.

The result for the aggregation of all substances s and compartments i, for a given time *t*, is obtained by:

$$n_{human}(t) = \sum_s \sum_i n_{human,s,i}(t) \quad (10)$$

$$n_{eco}(t) = \sum_s \sum_i n_{eco,s,i}(t) \quad (11)$$

The cumulated values, $n_{human,cumul}$ (cases) and $n_{eco,cumul}$ (PAF·m^3·day) for human toxicity and ecotoxicity can then be calculated:

$$n_{human,cumul}(TH) = \int_{t=t_0}^{TH} n_{human}(t) \quad (12)$$

$$n_{eco,cumul}(TH) = \int_{t=t_0}^{TH} n_{eco}(t) \quad (13)$$

where t_0 represents the time of the first emission into the environment and TH is the time span for which the cumulated impact is calculated.

It is worth noting that both dynamic approaches, climate change and toxicity, provide impact results at any point in time and are independent of the notion of time horizon – a key and controversial concept in conventional LCA.

2.2. Case study

In this work, a conventional wastewater treatment plant, WWTP, was used for a case study. The reason for this choice was the high variability of treatment conditions, leading to variable environmental interventions in time. The case study allowed a detailed analysis of the influence of temporal parameters on the dynamic impact results.

2.2.1. Goal and scope definition

A conventional and a dynamic LCA were performed and the results were compared for the target impact categories: climate change, human toxicity and ecotoxicity. Determining the sensitivity of the LCA results to temporal parameters was the main objective of this work.

The unit function was 1 m^3 of waste water treated respecting the regulatory rejection limits for the outlet effluent (water discarded into the environment) and the plant lifetime was taken as 30 years.

2.2.2. LCI

Fig. 2 shows the flowsheet of the WWTP studied. It comprised a primary clarification unit, 2 anoxic tanks and 3 aerobic tanks. A post denitrification zone was also added to achieve acceptable effluent quality. Nitrate was recycled from the aerobic to the anoxic zone. The sludge was separated in a secondary clarifier, which was also partly a wastage flow redirected to a thickener, and partly recycled in the anoxic zone. The resulting sludge was sent to incineration and the effluent discarded into the environment.

WWTP unit processes involve a large number of biological and chemical reactions with various dynamics. Modelling all the processes would be extensive and time consuming. For this reason, the dynamic simulation of the WWTP (the foreground process in LCA) was performed in Sumo® software, a wastewater treatment process simulator that includes biological, chemical, and physical processes. The database ecoinvent 3.2 was used for the background processes such as the production of raw materials, energy and infrastructure.

External carbon (methanol) was required to complete the denitrification, and iron chloride ($FeCl_3$) was added to chemically precipitate phosphorus in the sludge. Both additions were also necessary in order to satisfy legal discharge requirements for the effluent. The use of methanol releases carbon dioxide (CO_2), a percentage of which originates from a fossil source and should be taken into account in the inventory. Emissions of N_2O from WWTPs are considered to be 0.5% of nitrified ammonia flows in dynamic conditions (Czepiel et al., 1995). The volume and composition of off-gas were calculated (in Sumo® software) using gas/liquid transfer models. Calculations were based on transfer coefficients and concentration gradients with the atmosphere.

Heavy metal concentrations are not taken into account by Sumo® as these metals are considered to be inert for biological processes. Their input concentrations in WWTPs were therefore taken from Doka (2009) and Henze and Ledin (2001) and allocated to effluent and sludge in specific quantities, using the specific transfer coefficients proposed by the same authors.

The electricity consumption was calculated by taking the sum of all requirements: aeration of aerobic and nitrification tanks and thickener, mechanical mixing of anoxic tanks, pumping of main lines (influent input, dosing of chemicals, sludge output, recirculation lines, and effluent output), scraping and dewatering unit. Incineration of the sludge

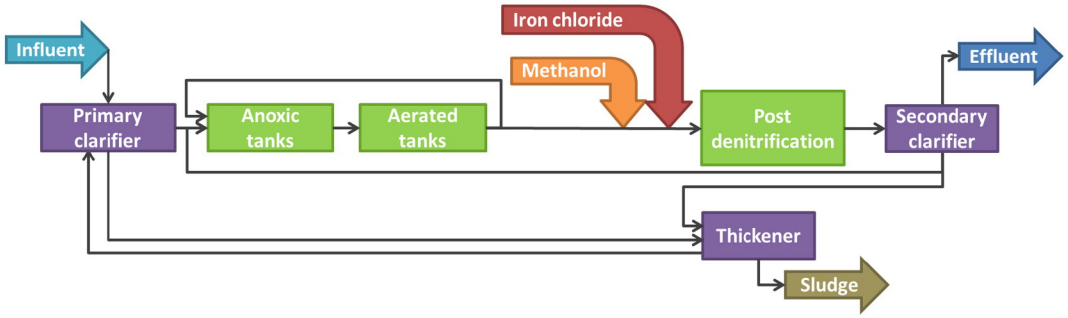

Fig. 2. Schema of the WWTP considered in the case study.

took account of gas-emissions in the form of CO_2, and metals (copper, lead and zinc).

WWTP basic infrastructure was included using a class 2 capacity data set from ecoinvent (which includes dismantling) and an annual sewage volume of approximately 1.4E7 m^3 was considered.

All inventory results are presented in SI, along with the ecoinvent reference for each flow.

2.2.3. Dynamic LCI

The flow rate and composition of the influent to a WWTP is commonly subject to time variations, i.e. low rate during the night and high rate during the day, weekend effect, influence of holidays, and seasonal effects (Gernaey et al., 2011) (flow variations presented in SI). In order to include these variations in the plant dynamic model, the influent generator of Gernaey et al. (2011) was used. Thus, it was considered that the operation of the plant and the influent it received had variable and cyclic behaviour with a period of 1 year. Consequently, the inventories of the foreground processes (direct emissions of CO_2, CH_4 and N_2O by the plant; CO_2, N_2O, heavy metals and organic substances from sludge treatment) and of the supply chain (iron chloride, methanol and electricity consumption) were also variable. The variations of emissions in the WWTP were calculated with Sumo® for the interval of one year and the results were replicated for every year of its life span.

Raw materials (methanol, iron chloride) were considered to be supplied every 2 months (delay of 60 days and production period of 1 day). Electricity was considered to be supplied continuously during the life time of the WWTP. The time considered for the infrastructure construction of the WWTP was 3 years for the processes of building and 6 months' delay for the plant start up. The temporal parameters used for the background processes are shown in SI. The temporal behaviour of the background environmental interventions was calculated with the web-tool DyPLCA (Tiruta-Barna et al., 2016).

The inventory results obtained with Sumo and DyPLCA are in the form of discrete values in time for a predefined time step of 0.5 days. This time step corresponds to the smallest duration for a significant variation of physical parameters involved in the WWTP operation (variation of the influent flow rate for instance). Coarser time granulometries can also be used, for capturing daily, monthly or seasonal variations. Consequently, additional time step sizes were analysed: 1 day, 1 week, 1 month, 1 season and 1 year. The discrete values of the initial dynamic inventory were thus recalculated for each time granulometry:

$$g_s(t)_{\Delta t_{higher}} = \frac{1}{\Delta t_{higher}} \sum_{t'=n}^{n+m-1} g_s(t')_{\Delta t_{lower}} \Delta t_{lower} \quad (14)$$

$$for\ n = (t_0, t_0 + m, t_0 + 2m, \ldots, t_{final})\ and\ m = \frac{\Delta t_{higher}}{\Delta t_{lower}}$$

where t is the discrete time value for the new time scale granulometry; t′ is the discrete time value in the initial LCI time scale (step size of 0.5 days); s is the substance being analysed, t_{final} is the discrete time at which the last emission of the dynamic inventory is released (day); $g_s(t')$ is the mass flow value for a specific substance and for a specific time t′, which is the result of the dynamic LCI ($kg \cdot day^{-1}$), Δt_{lower} is the time step used for the calculation of the dynamic LCI (i.e. 0.5 days), Δt_{higher} is the new time step required and t_0 is the initial time in the dynamic LCI.

In this way, the same total quantity of a substance can be differently distributed in time (with different granulometries), leading to different profiles of the dynamic LCI, $g_s(t)$.

Conventional LCI values, $g_{s,total}$ (kg), can be retrieved by the time integration of the dynamic LCI:

$$g_{s,total} = \int_{t=t_0}^{t_{final}} g_s(t)dt \quad (15)$$

2.2.4. LCIA

The impact categories chosen in this study are those for which a dynamic approach exists, as presented in Section 2.1. The IPCC climate change and USEtox toxicity models are the basis of the dynamic impact models and were also used in conventional LCA applied to the case under study.

A calculation time span of 100 years was chosen for both dynamic impacts. In conventional LCA, a time horizon of 100 years is commonly used for climate change while, for toxicity categories steady state condition equivalent to an indefinite time horizon is considered.

2.3. Sensitivity analysis

Dynamic inventory results represent the emission variations due to the behaviour of the supply chain and processes. Moreover, dynamic impact assessment is based on environmental models that can be sensitive to different time scales (days, months, years, decades, etc.). One of the major questions subsequent to a time dependent approach of LCA concerns the extent to which the temporal parameters influence the LCA results and, in particular, how the time granulometry used in the definition of the dynamic flows will affect the temporal profile of the calculated impacts.

To investigate this, the influence of each of the following parameters was analysed: i) the detail of the temporal definition of the inventory (a process and supply chain characteristic), ii) the calculation time span (time horizon in conventional LCA) for the dynamic impact methods, iii) the time step size resolution of the dynamic impact models (including the ODE specifications).

For this study, several emissions from the system's life cycle were selected based on a significant variation in their temporal profile, and also based on their important contribution to the LCA results as pointed out by previous studies (Bisinella de Faria et al., 2015; Bisinella de Faria et al., 2016). In this sense, CO_2, CH_4 and N_2O were considered as they are direct emissions from the WWTP, from sludge incineration and from the infrastructure processes. Metals emitted by sludge incineration (copper, zinc, lead, chromium, mercury) and infrastructure processes (mercury) were analysed, all of them being included in the USEtox database. Phenomenological parameters inherent to the LCIA models had already been investigated for climate change and toxicity in other studies (IPCC, 2013; Henderson et al., 2011; Rosenbaum et al., 2011) and were not analysed in this work.

Several approaches exist for sensitivity analysis, such as variance decompositions, partial derivatives or elementary effects. A one-at-a-time sensitivity method was used, i.e. the effects of only one parameter were investigated at a time. The sensitivity indicator is the relative difference between the impact results of a given scenario (with a modified parameter) and the reference scenario (reference values for the temporal parameters), calculated by:

$$\text{relative difference}\ (t) = \frac{n(t)_{step} - n(t)_{step}^{ref}}{n(t)_{step}^{ref}} \quad (16)$$

where $n(t)_{step}$ is the impact value at time t for the calculation scenario with a variable temporal parameter 'step' (e.g. LCI time step size), 'ref' indicates the reference calculation scenario with predefined values for the temporal parameters (e.g. LCI time step of 1 year).

3. Results and discussion

3.1. Influence of the dynamic LCI profile and the time span of the impact calculation

LCI results for different time steps are available for all the substances selected in this work. The mass balance was verified by calculating the cumulated inventory $g_{s,total}$ per substance. Table 1 shows that the values

Table 1
Cumulated LCI results for WWTP case study calculated with different time step sizes (0.5 day, 1 day, 1 week, 1 month, 1 season and 1 year).

	Carbon dioxide	Methane	Dinitrogen monoxide	Copper	Lead	Zinc	Copper
0.5 day	9.5E-02	2.1E-04	2.9E-06	2.0E-06	1.9E-06	1.1E-05	2.1E-08
1 day	9.5E-02	2.1E-04	2.9E-06	2.0E-06	1.9E-06	1.1E-05	2.1E-08
1 week	9.5E-02	2.1E-04	2.9E-06	2.0E-06	1.9E-06	1.1E-05	2.1E-08
1 month	9.5E-02	2.1E-04	2.9E-06	2.0E-06	1.9E-06	1.1E-05	2.1E-08
1 season	9.5E-02	2.1E-04	2.9E-06	2.0E-06	1.9E-06	1.1E-05	2.1E-08
1 year	9.5E-02	2.1E-04	2.9E-06	2.0E-06	1.9E-06	1.1E-05	2.0E-08

	Lead	Zinc	Methylene chloride	Chloroform	Chromium III	Mercury
0.5 day	2.0E-08	1.2E-07	7.9E-08	1.7E-07	3.3E-09	2.9E-11
1 day	2.0E-08	1.2E-07	7.9E-08	1.7E-07	3.3E-09	2.9E-11
1 week	2.0E-08	1.2E-07	7.9E-08	1.7E-07	3.3E-09	2.9E-11
1 month	2.0E-08	1.1E-07	7.9E-08	1.7E-07	3.3E-09	2.9E-11
1 season	2.0E-08	1.2E-07	7.9E-08	1.7E-07	3.3E-09	2.9E-11
1 year	2.0E-08	1.1E-07	7.8E-08	1.7E-07	3.3E-09	2.9E-11

do not present any great variation when the step size is changed. The calculation of the relative difference between the cumulated values for different step sizes and the reference (time step size of 1 year) did not exceed 1%. These results are in accordance with the mass balance, which does not change with the calculation time step.

3.1.1. Climate change results

Fig. 3 shows the dynamic LCI results for the emission of carbon dioxide in kg.day^{-1} during the life cycle of the WWTP studied. The different graphics of Fig. 3 were obtained for LCI time step sizes of 0.5 day, 1 day, 1 week, 1 month, 1 season and 1 year.

Fig. 3.A, B and C show the important influence of the variation of emissions due to the different temporal characteristics of the process. On the other hand, the profile of emissions represented in the graphics 3.D, E and F tend to a constant value around 3.3E-3 kg·day^{-1}, representing almost steady state conditions. For this reason, the calculation scenario with the time step of 1 year was chosen as the reference calculation scenario (ref in Formula 16). The maximum time step for which the inventory variations can be clearly distinguished is a week for this case study. The amplitude of the emissions also change: the values for the emissions in Fig. 3.A range between 0 and 0.06 kg·day^{-1} while they range only between 0.001 and 0.01 kg·day^{-1} in Fig. 3.C.

Fig. 4 shows the comparison between the results for dynamic mean temperature change and cumulated radiative forcing, calculated with different inventory step sizes (0.5 day, 1 day, 1 week, 1 month, 1 season and 1 year) for a time span of 100 years. Carbon dioxide, methane and dinitrogen monoxide were considered. The step size used for the calculation of the dynamic climate change impact was 0.5 days.

No noteworthy difference could be seen between the curves corresponding to the dynamic method, highlighting the low response of the climate change model (both indicators) to the temporal variations of emissions at daily to monthly levels.

Table 2 details the relative difference between the values calculated with the dynamic model for different LCI time step sizes and the case when step size was 1 year. The case of step size of 1 year is considered as the reference since the plant behaves as steady state system with constant emissions. The values of dynamic impact for both climate change indicators were calculated at year 100. At this time point, they did show a marked difference when the LCI step size was modified.

As expected, the lower the time step size, the higher the relative difference (with respect to the steady state emission) in the climate change results. However, these results show that the dynamic model

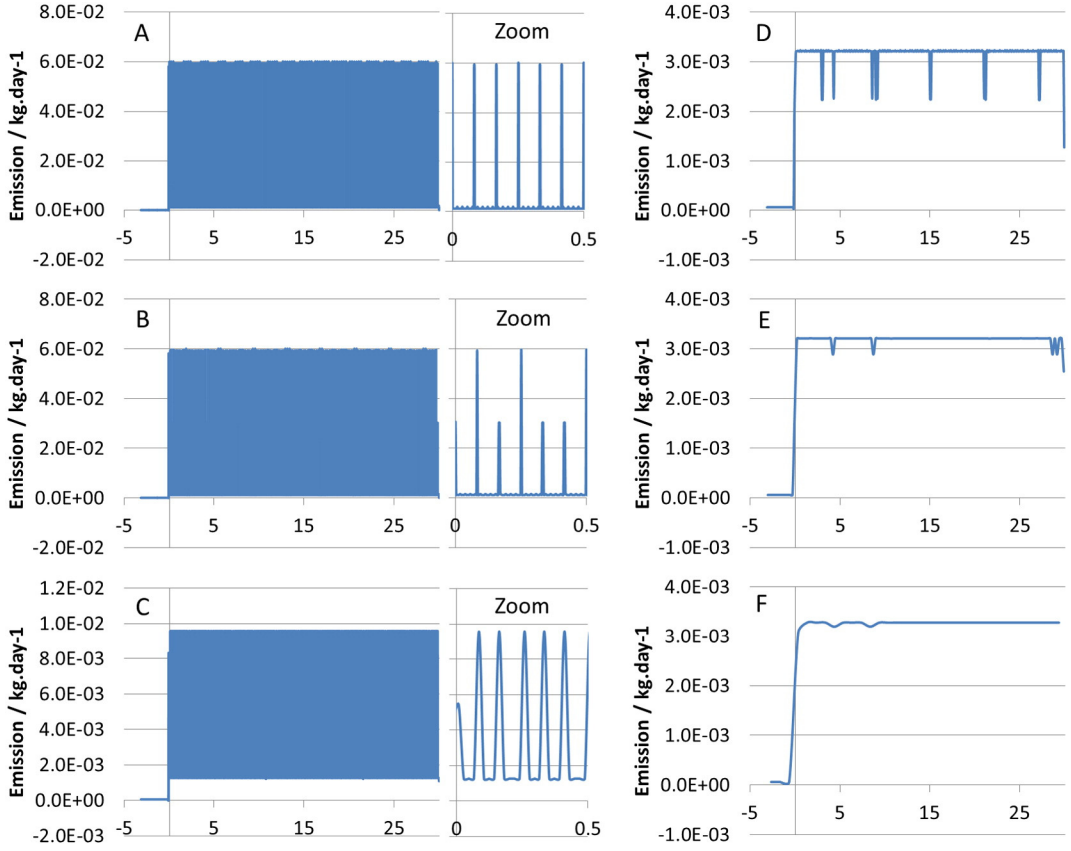

Fig. 3. CO_2 emission by the life cycle system of a WWTP. Dynamic inventory for different time step sizes (A - 0.5 day, B - 1 day, C - 1 week, D- 1 month, *E*- 1 season and F- 1 year). Zoom on the year between 0 and 0.5 for A, B and C.

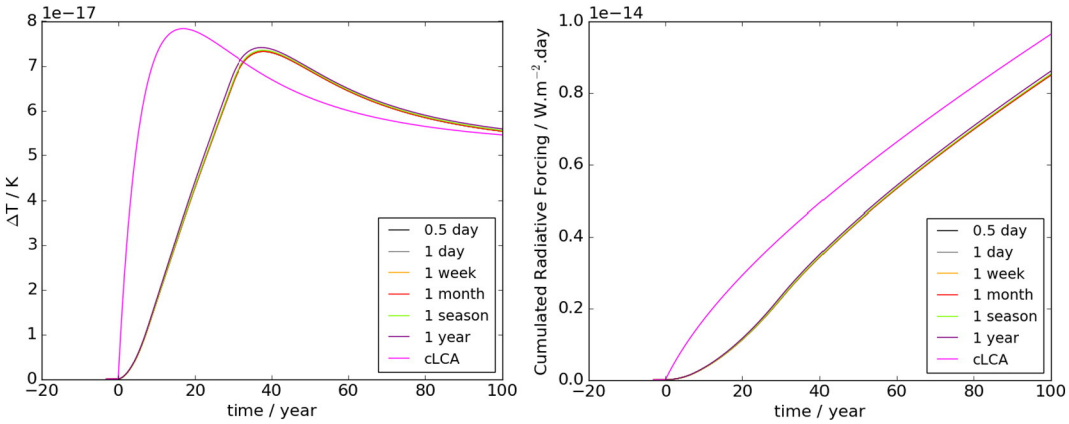

Fig. 4. – Mean temperature change and cumulated radiative forcing for the case study of the WWTP, calculated for a time span of 100 years. Dynamic LCI inventory step sizes analysed: 0.5 day, 1 day, 1 week, 1 month, 1 season and 1 year. Results for conventional methods: cLCA curve.

Table 2
Relative difference of mean temperature change and cumulated radiative forcing for a time span of 100 years. The reference is the case of LCI time step size of 1 year. LCI time step sizes of 0.5 day, 1 day, 1 week, 1 month and 1 season were analysed.

Substance	Relative difference of ΔT results at year 100 (K)				
	0.5 day	1 day	1 week	1 month	1 season
Carbon dioxide	−1.2%	−1.2%	−1.2%	−1.1%	−0.8%
Methane	−0.6%	−0.6%	−0.5%	−0.4%	−0.3%
Dinitrogen monoxide	−1.1%	−1.1%	−1.1%	−1.0%	−0.8%
All substances	−1.2%	−1.2%	−1.2%	−1.1%	−0.8%
Substance	Relative difference of cumulated radiative forcing results at 100 years (W·m^{-2}·day)				
	0.5 day	1 day	1 week	1 month	1 season
Carbon dioxide	−1.6%	−1.6%	−1.5%	−1.4%	−1.1%
Methane	−1.2%	−1.2%	−1.1%	−1.0%	−0.8%
Dinitrogen monoxide	−1.5%	−1.6%	−1.5%	−1.5%	−1.1%
All substances	−1.3%	−1.3%	−1.3%	−1.3%	−0.9%

is not significantly sensitive to the time step size of LCI (at least for the present case study and similar systems) at any time. This allows a higher time step size to be used in the dynamic inventory calculation, which is more practical and easier to obtain, and requires less computational work and time.

Regarding the conventional mean temperature change in Fig. 4 (left side), this method considers that all the emission occurs at time zero. The maximum value for mean temperature change is higher for the conventional method than for the dynamic method. The conventional method gives a maximum value of 7.8E-17 K and it is reached by year 16. For the dynamic method, the maximum value is 7.4E-17 K by year 37. The result obtained at year 100 is similar for both methods, presenting a value of around 5.5E-17 K. The cumulated radiative forcing is the impact indicator in the conventional climate change impact method. In Fig. 4 (right), the values attained at year 100 are around 8.5E-15 W·m^{-2}·day for the dynamic method and 9.6E-15 W·m^{-2}·day for the conventional method. The difference between dynamic and conventional results is almost constant during the whole calculation period, showing that the conventional calculation overestimates the impact from the beginning.

Table 3 shows the mean temperature change and cumulated radiative forcing values for the WWTP case study at a time span of 100 years. It also shows the relative difference between dynamic and conventional values in parentheses. Considering the mean temperature change for a time span (or time horizon) of 100 years, methane

Table 3
Dynamic and conventional climate change (cLCA) values (mean temperature change and cumulated radiative forcing) for a time span of 100 years. In parentheses are the relative differences between conventional and dynamic values.

Substance	Mean ΔT value at year 100 (K)						
	Dynamic inventory step size						cLCA
	0.5 day	1 day	1 week	1 month	1 season	1 year	
Carbon dioxide	5.3E-17 (2.3%)	5.3E-17 (2.3%)	5.3E-17 (2.4%)	5.4E-17 (2.5%)	5.4E-17 (2.8%)	5.4E-17 (3.6%)	5.2E-17
Methane	5.7E-19 (19.3%)	5.7E-19 (19.3%)	5.7E-19 (19.4%)	5.7E-19 (19.6%)	5.7E-19 (19.6%)	5.8E-19 (20.0%)	4.8E-19
Dinitrogen monoxide	4.1E-19 (9.3%)	4.1E-19 (9.3%)	4.1E-19 (9.3%)	4.1E-19 (9.4%)	4.1E-19 (9.7%)	4.1E-19 (10.5%)	3.7E-19
All substances	5.4E-17 (2.5%)	5.4E-17 (2.5%)	5.4E-17 (2.6%)	5.4E-17 (2.7%)	5.5E-17 (3.0%)	5.5E-17 (3.8%)	5.3E-17
	Cumulated radiative forcing at 100 years (W·m^{-2}·day)						
	0.5 day	1 day	1 week	1 month	1 season	1 year	cLCA
Carbon dioxide	7.7E-15 (−12.0%)	7.7E-15 (−12.0%)	7.7E-15 (−12.0%)	7.7E-15 (−11.9%)	7.7E-15 (−11.6%)	7.8E-15 (−10.6%)	8.8E-15
Methane	5.3E-16 (−0.6%)	5.3E-16 (−0.6%)	5.3E-16 (−0.5%)	5.3E-16 (−0.4%)	5.3E-16 (−0.2%)	5.4E-16 (−0.6%)	5.4E-16
Dinitrogen monoxide	6.3E-17 (−10.8%)	6.3E-17 (−10.9%)	6.3E-17 (−10.8%)	6.4E-17 (−10.7%)	6.4E-17 (−10.5%)	6.4E-17 (−9.4%)	7.1E-17
All substances	8.5E-15 (−9.3%)	8.5E-15 (−9.3%)	8.5E-15 (−9.3%)	8.5E-15 (−9.3%)	8.5E-15 (−8.9%)	8.6E-15 (−8.1%)	9.4E-15

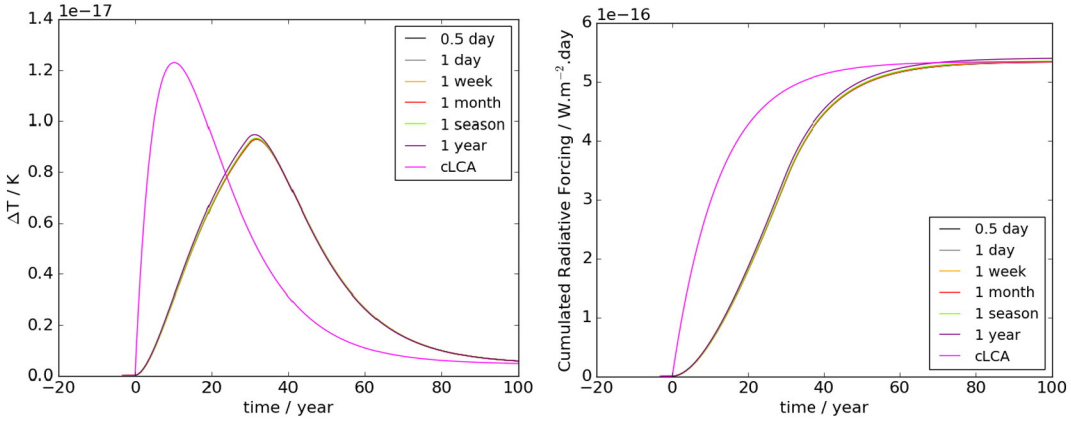

Fig. 5. – Mean temperature change and cumulated radiative forcing for methane calculated for a time span of 100 years. Dynamic LCI inventory step sizes analysed: 0.5 day, 1 day, 1 week, 1 month, 1 season and 1 year. Results for conventional method: cLCA curve.

presented a large difference, of about 20%, between the conventional and dynamic results. On the other hand, the relative difference between the conventional and dynamic mean temperature change values for carbon dioxide was quite small, about 3%.

Considering the comparison between the dynamic and conventional cumulative radiative forcing, there is almost no difference for the methane results. On the other hand, dinitrogen monoxide and carbon dioxide present large differences. The global cumulated radiative forcing is higher in conventional LCA than in the dynamic approach, which signifies that, for a time horizon of 100 years, conventional LCA overestimates the climate change impact.

Table 3 also points out that the values obtained for all substances taken together are very close to the values obtained for CO_2, which is explained by the fact that CO_2 is the major GHG in this case study. Obviously this behaviour cannot be generalized.

In order to flesh out the results observed above, Fig. 5 shows the results obtained for methane with the same calculation conditions as for Fig. 4. Here too, no important difference can be seen between the curves obtained for various inventory time step sizes. The maximum value for mean temperature change is higher for the conventional method than for the dynamic method. It has a value of 1.2E-17 K, which is reached by year 10. For the dynamic method, the maximum value is 9.5E-18 K by year 30. Both curves tend towards a low limit as methane has a limited lifetime in the atmosphere and is transformed into CO_2.

Figs. 4 and 5 clearly show that the effects in terms of mean temperature change and cumulated radiative forcing have amplitudes and

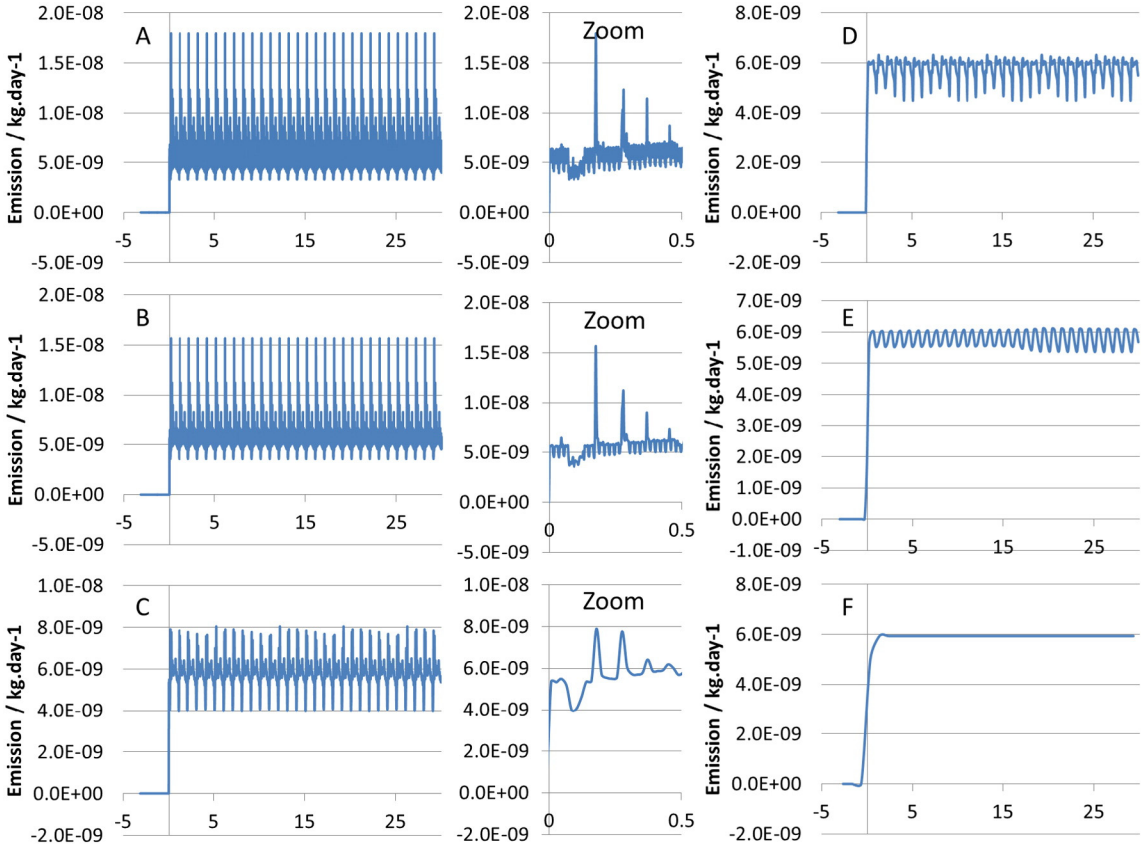

Fig. 6. – Chloroform emission by the life cycle system of a WWTP. The dynamic inventory was calculated for different time step sizes (A - 0.5 day, B - 1 day, C - 1 week, D- 1 month, E- 1 season and F- 1 year) and zooms are presented for the time between 0 and 0.5 years in A, B and C.

positions on the time scale that depend on the GHG emission duration and time position, and on the lifetime of each GHG. In conventional LCA, all information related to the time occurrence of the (worst) effects, at the human time scale of about 100 years, is lost by the zero time point emission on one hand, and by an arbitrarily chosen time horizon on the other. For industrial processes with lifetimes of about 20–30 years, a time horizon of 100 years (or any other fixed value) is not suitable. Instead, dynamic methods offer the possibility of monitoring the climate change indicators over time.

3.1.2. Toxicity results

Fig. 6 shows the dynamic LCI results for the emission of chloroform in kg·day^{-1} during the life cycle of the WWTP studied. The different graphics of Fig. 6 were obtained for step sizes of 0.5 day, 1 day, 1 week, 1 month, 1 season and 1 year.

Chloroform emission was directly linked to the effluent flow, which presents seasonal effects during the year. Among the organic compound released, chloroform had the major influence on the toxicity. The maximum amplitude of the emissions is observed for the smallest time step (0.5 days) in Fig. 6.A. It ranges between 4*E*-9 and 1.8E-8 kg.day^{-1}.

Figs. 7 and 8 show the results for the current ecotoxicity, $n_{eco}(t)$, and human toxicity, $n_{human}(t)$, calculated over 100 years with the dynamic approach.

In Fig. 7 current human toxicity and ecotoxicity were calculated separately for organic (non persistent) compounds and inorganic (persistent) substances. The origin of the different behaviours observed for these two groups of substances was previously discussed (Shimako et al., 2017). Fig. 7 was obtained by simulations using a time step size of 1 day for the temporal LCI definition. As chloroform is the major contributor, the results in graphics A are dominated by chloroform's behaviour. The toxicity temporal profile follows the emission profile (Fig. 6 – B: time step 1 day) in terms of periodicity and regularity of amplitudes. Overall, inorganic substances (Fig. 7 – B) seemed to dominate the results, the toxicity values being of several orders of magnitude higher than those of organics.

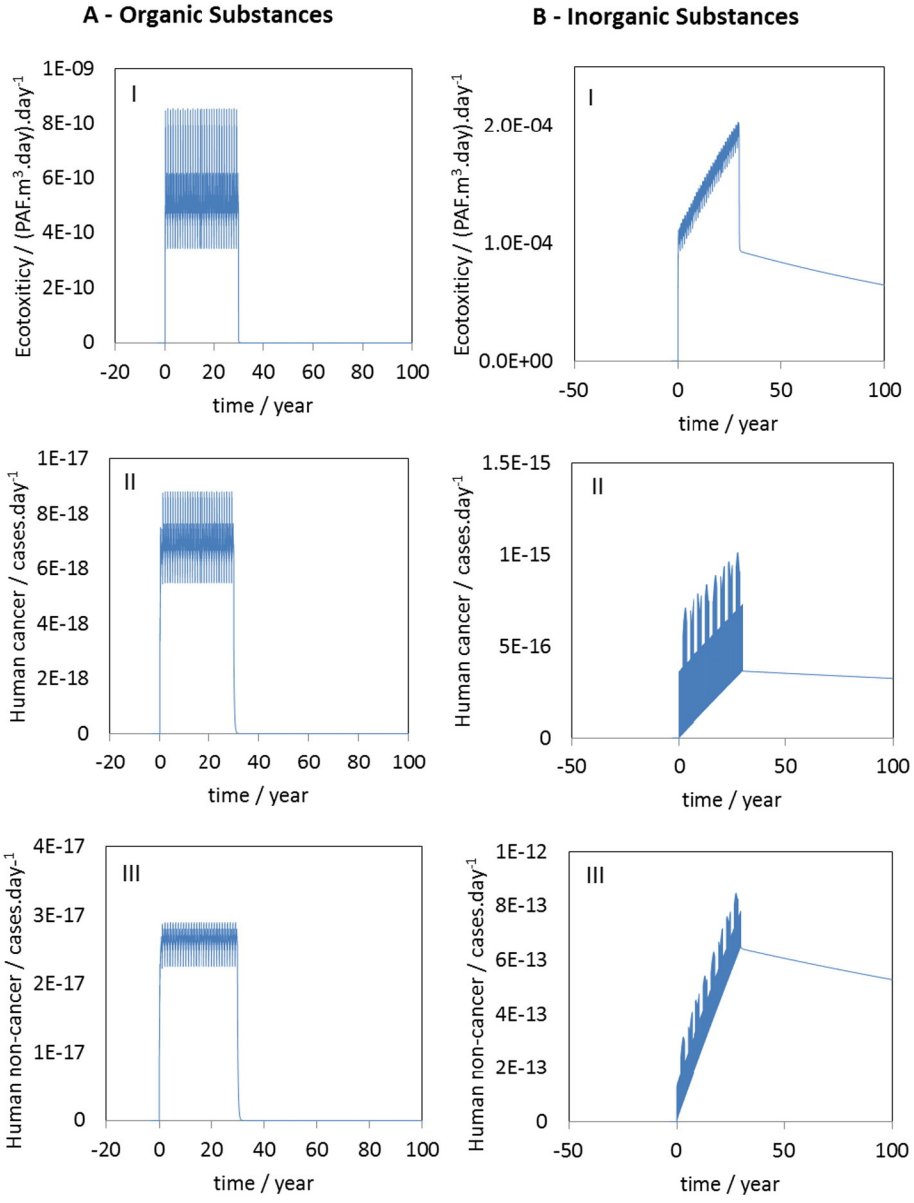

Fig. 7. Current toxicity (cancer: graphics II, non-cancer: graphics III) and ecotoxicity (graphics I). Calculation for all organic substances: graphics A (left side of the figure), and for all inorganic substances: graphics B (right side of the figure).

A more detailed analysis was performed on the global results obtained for all substances selected for the case study. In Fig. 8 different time step sizes (0.5 day, 1 day, 1 week, 1 month, 1 season and 1 year) were used in the calculation of the dynamic inventory, which was the input to the dynamic toxicity model. The time step size used to retrieve toxicity results (from the toxicity model calculation) was the lowest one investigated, i.e. 0.5 day.

Ecotoxicity results present slight differences between the amplitudes and temporal profile of the impacts calculated with different step sizes. The difference of amplitudes is much greater for both cancer and non-cancer human toxicity results. The observed differences of amplitudes and temporal profiles in the dynamic toxicity results are the direct reflection of the substance emission behaviour of the life cycle system and thus of the dynamic LCI. This aspect has already been pointed out by Shimako et al. (2017).

Fig. 9 shows the relative difference between the results for dynamic toxicity (all substances) calculated with different step sizes compared

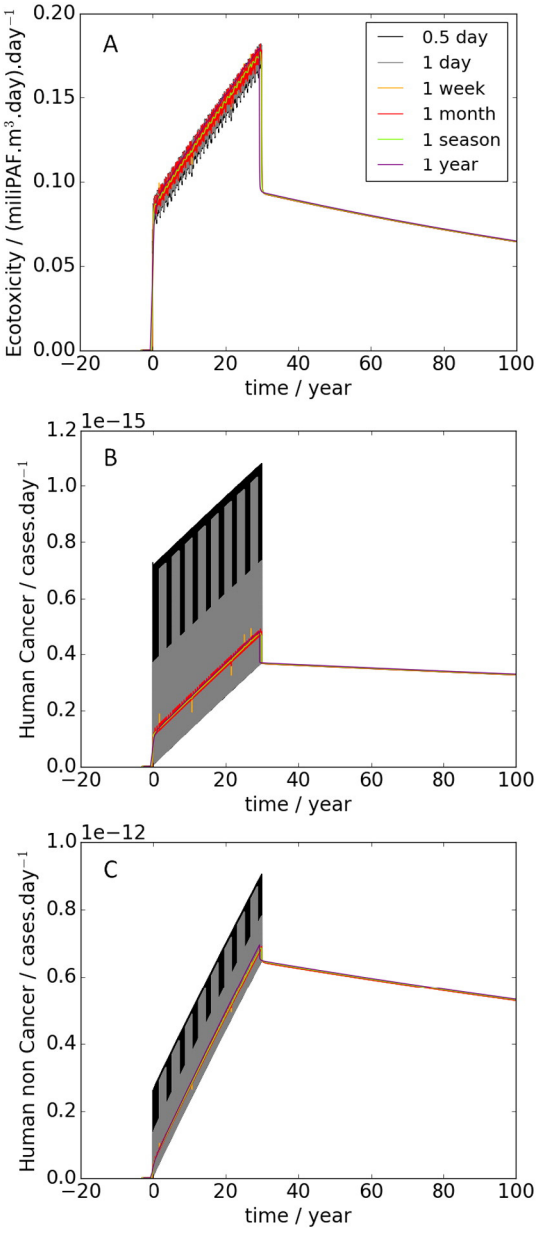

Fig. 8. - Ecotoxicity (A), human cancer toxicity (B) and human non-cancer toxicity (C) for the case study (all substances) calculated over 100 years, for different time step sizes in the LCI.

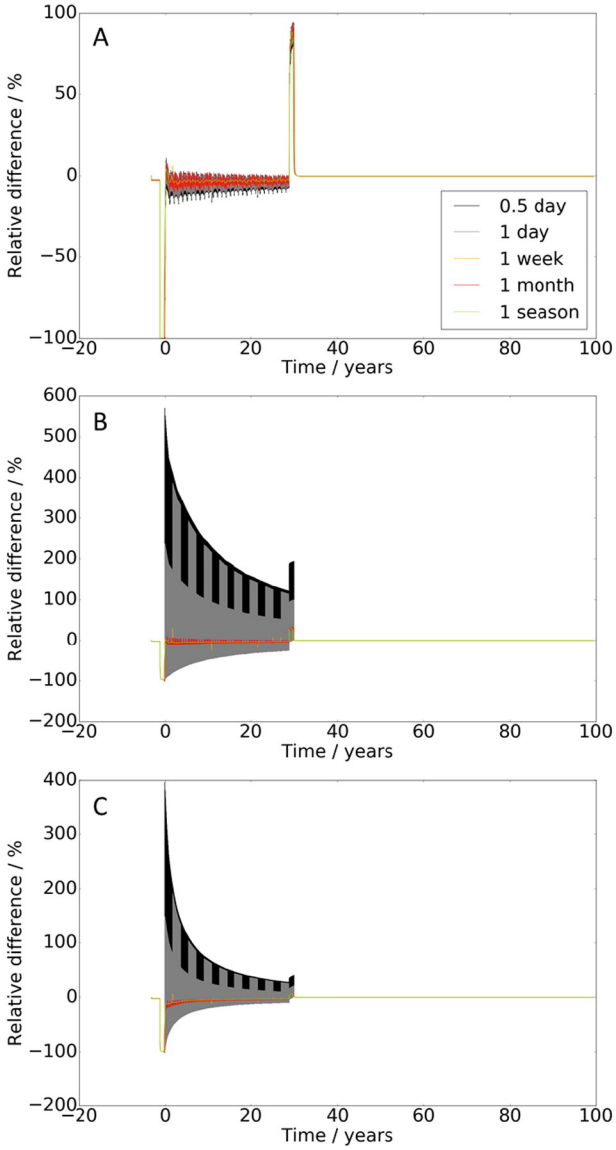

Fig. 9. Relative difference for current ecotoxicity (A), human cancer toxicity (B) and human non-cancer toxicity (C), calculated with the dynamic approach for a time span of 100 years. Reference step size = 1 year. Step sizes analysed: 0.5 day, 1 day, 1 week, 1 month and 1 season.

with the reference result (step size of 1 year). The most spectacular differences are observed for human toxicity. The profiles calculated for 0.5 and 1 day present significantly higher amplitudes than those obtained with other time step sizes. The relative difference for ecotoxicity is much smaller. Two distinct high amplitudes were obtained, one by year 0 and the other by year 30 but this is, in fact, an artefact attributable to the numerical integration method (Eq. 14).

Table 4 shows the results of dynamic cumulated toxicity at 100 years, and the relative difference with respect to the conventional LCA results. In a previous study (Shimako et al., 2017), it was demonstrated that toxicity impacts due to non-persistent (organic) and persistent (mostly inorganic) substances had very different temporal profiles. For that reason, in the present work, calculations were performed considering all substances, or only organic substances, or only inorganic substances.

Differences between the dynamic approach and conventional LCA are very significant for “all substances” and “inorganic substances”, reaching 85% in the human cancer toxicity category. In contrast, relative differences are insignificant for “organic substances” at the chosen time

span of 100 years. The concentration of non-persistent organic substances in all environmental media tends to zero by year 100, while inorganics persist and generate more and more cumulated impact. As conventional LCA considers steady sate conditions (theoretically reached for constant emissions over very long time frames), i.e. an infinite time horizon, the conventional toxicity method overestimates the effect of inorganic substances. The dynamic approach provides much more realistic results at a given moment on the time scale. Indeed, the contribution of sink reservoirs in the Simplebox model (substance degradation and removal) is much more influent in real systems and dynamic conditions (emissions taking place over a limited duration) as in the theoretical "ideal" condition of continuous constant emission over infinity.

Moreover, the LCI time step size is not a sensitive parameter when the dynamic and conventional results are compared since the observed gap is dominated by the predefined time horizon of infinity.

It can be concluded that current dynamic toxicity exhibits a temporal profile with marked variations and large amplitude differences when distinct LCI time step sizes are used. For all toxicity categories, the relative difference (between curves with different time step sizes) vanishes after the life time of the system, i.e. 30 years. At 100 years, the values of cumulated dynamic toxicities, calculated with different LCI time step sizes, are much the same (the relative differences between the reference case and the others do not exceed 1.7% - see SI). The temporal variation of the potential toxicity impact (cases·day^{-1}) and thus the most relevant point in time for the assessment is information that is inaccessible in the conventional method.

3.2. Influence of the time step of the dynamic impact model resolution

3.2.1. Climate change

The variation on the dynamic LCI step size (Section 3.1) showed that there was no significant difference in the climate change results, for the mean temperature change, when calculations were performed with time steps from 0.5 day to 1 year. Using a 1 year step size for the inventory allows different step sizes (less than 1 year) to be used for the calculation of the dynamic climate change impact. The calculation was done for the dynamic LCIA step size of 0.5 day, 1 day, 1 week, 1 month, 1 season and 1 year.

The three main GHG were considered in this analysis (carbon dioxide, methane and dinitrogen monoxide). A time step greater than 1 year was not envisaged in the present case study as it would have neglected some discrete mass values from the dynamic inventory.

Table 5 shows the relative difference between the results obtained for the mean temperature change with different time step sizes. The relative difference is not significant for step sizes in the interval of 0.5 day to 1 season. However, the result obtained with a step size of 1 year shows differences of about 5%. Considering that the smallest time step size gives the most precise results, this means that any step between 0.5 days and 1 season can be used, given the insignificant difference between the results.

In this work, a personal computer with an Intel Core i5-2540 M processor at 2.60 GHz and 4 GB of RAM was used. Even though the computer can support multithread, only a single core was used for the computation. The calculation time decreased substantially when the

Table 5
– Relative difference for mean temperature change, obtained for different time step sizes in the climate change model resolution.

Relative difference for ΔT	0.5 day	1 day	1 week	1 month	1 season	1 year
0.5 day	0.0%	0.0%	0.0%	−0.1%	−0.4%	−5.2%
1 day	–	0.0%	0.0%	−0.1%	−0.4%	−5.2%
1 week	–	–	0.0%	−0.1%	−0.4%	−5.1%
1 month	–	–	–	0.0%	−0.3%	−5.0%
1 season	–	–	–	–	0.0%	−4.8%
1 year	–	–	–	–	–	0.0%
Calculation time	9 h 34 m 30 s	2 h 23 m 20 s	3 m	15 s	6 s	8 s

Table 4
Cumulated values for dynamic toxicity impact calculated over 100 years and values for conventional LCA (cLCA). Relative difference between dynamic and conventional results is given in parentheses.

	All substances						
	0.5 day	1 day	1 week	1 month	1 season	1 year	cLCA
Ecotoxicity (PAF·m^3·day)	3.1E+00 (56.5%)	3.1E+00 (56.5%)	3.1E+00 (56.4%)	3.1E+00 (56.4%)	3.1E+00 (56.2%)	3.1E+00 (55.8%)	7.1E+00
Human cancer (cases)	1.1E-11 (85.6%)	1.1E-11 (85.6%)	1.1E-11 (85.6%)	1.1E-11 (85.6%)	1.1E-11 (85.5%)	1.2E-11 (85.3%)	7.8E-11
human non –cancer (cases)	1.7E-08 (80.9%)	1.7E-08 (80.9%)	1.7E-08 (80.9%)	1.7E-08 (80.9%)	1.7E-08 (80.8%)	1.7E-08 (80.6%)	8.9E-08
	Organic substances						
	0.5 day	1 day	1 week	1 month	1 season	1 year	cLCA
Ecotoxicity (PAF.m^3.day)	2.8E-06 (−0.3%)	2.8E-06 (−0.3%)	2.8E-06 (−0.3%)	2.8E-06 (−0.3%)	2.8E-06 (−0.6%)	2.8E-06 (−1.1%)	2.7E-06
Human cancer (cases)	3.7E-14 (0.2%)	3.7E-14 (0.2%)	3.7E-14 (0.2%)	3.7E-14 (0.2%)	3.7E-14 (0.1%)	3.8E-14 (−0.6%)	3.7E-14
human non –cancer (cases)	1.4E-13 (0.0%)	1.4E-13 (0.0%)	1.4E-13 (0.0%)	1.4E-13 (0.0%)	1.4E-13 (0.4%)	1.4E-13 (0.8%)	1.4E-13
	Inorganic substances						
	0.5 day	1 day	1 week	1 month	1 season	1 year	cLCA
Ecotoxicity (PAF·m^3·day)	3.1E+00 (56.5%)	3.1E+00 (56.5%)	3.1E+00 (56.4%)	3.1E+00 (56.4%)	3.1E+00 (56.2%)	3.1E+00 (55.8%)	7.1E+00
Human cancer (cases)	1.1E-11 (85.6%)	1.1E-11 (85.6%)	1.1E-11 (85.6%)	1.1E-11 (85.6%)	1.1E-11 (85.5%)	1.1E-11 (85.4%)	7.8E-11
human non –cancer (cases)	1.7E-08 (80.9%)	1.7E-08 (80.9%)	1.7E-08 (80.9%)	1.7E-08 (80.8%)	1.7E-08 (80.8%)	1.7E-08 (80.6%)	8.9E-08

step size for the convolution calculation was increased, because of the number of iterations required by a convolution product (Garge and Shirali, 2012):

$$iterations = \frac{number\ of\ discretizations\ (number\ of\ discretizations + 1)}{2} \quad (17)$$

As the difference between the results is not substantial, a time step size of 1 month or 1 season could be envisaged for the calculation and would provide a good compromise between accuracy of results and computational efficiency.

3.2.2. Toxicity

A similar comparison between different step sizes was not possible in the dynamic toxicity model because the dynamic toxicity results are, first of all, very sensitive to the time step size of the inventory. Calculation of dynamic toxicity using a 1 year step size for the dynamic inventory is not suitable as it does not consider all the potential variations and amplitudes of the toxicity impact. Moreover, it has been shown (Shimako et al., 2017) that the resolution of the dynamic toxicity model depends on the resolution of an ODE, which requires an adaptive integration time step. Thus, the lower the time step is, the more reliable is the dynamic impact profile and the more accurate is the numerical resolution. It is, however, possible to set the maximum step for the ODE solver in the toxicity model at the LCI step size, e.g. 0.5 days.

4. Conclusion

The dynamic LCA framework presented here combined the DyPLCA inventory model with dynamic climate change and dynamic toxicity impact assessment models. Sensitivity analysis was conducted on a case study in order to identify the influence of the temporal profile of the dynamic LCI and of the time horizon on the final LCA results. Additionally, parameters of numerical methods used for the resolution of the impact models were investigated.

As a general remark, both impact categories exhibit high variation over the calculation period (100 years in this study), which cannot be captured in a single impact value at a given time (or a fixed time horizon), e.g. 100 years. Instead, a detailed analysis is necessary during the first few decades. In this case, a graphical representation of the LCA results is of great interest for the identification of the general temporal profile. The subsequent conclusion is that a fixed time horizon, as implemented in conventional LCA, deprives us of essential information, especially for short and medium time periods corresponding to the lifetime of the studied system and about the following twenty years.

For climate change impact, two dynamic indicators were analysed: the global mean temperature change and the cumulated radiative forcing. The temporal profile of both indicators depends on the target substance and the global positioning of the GHG emissions on the time scale, i.e. emission beginning and duration. In consequence, a fixed time horizon as in conventional LCA is highly arbitrary and does not correspond to any point of interest on the time scale of the processes, i.e. temporal LCI and dynamic phenomena involved in impact deployment.

In this work it is shown that neither dynamic indicator is sensitive to the level of detail of the temporal LCI definition. Simulations performed for the same process system, but varying the granulometry of the LCI from 0.5 day to 1 year, led to similar results.

The dynamic climate change model is not sensitive to the change of time step size for numerical resolution, on condition that it lies below the LCI time step size (otherwise inventory information can be lost). For the case study, a time step of 1 month satisfied the resolution accuracy condition, for a very reasonable computational effort.

The dynamic toxicity model was based on USEtox model parameters. As in the case of climate change, the toxicity temporal profile depends on the target substance and temporal definition of LCI. However, unlike for climate change, in the case of toxicity, the level of detail of the LCI definition (time granulometry) has a major influence on the results: toxicity results are highly sensitive to the LCI time step. The time step size of the temporal LCI definition is intrinsically linked to the behaviour of the studied system and should not be chosen by the LCA practitioner. However, if a choice is possible, the smallest time step for toxicity assessment is advised.

Concerning the time span of calculation, as in the case of climate change, there is no justification for fixing a predefined value. In conventional LCA, the fate of substances in the environment is considered to be at steady state, i.e. the time horizon is undefined and sink processes are compensated by the continuous infinite emission. However, it is shown here that the most interesting period is the lifetime of the studied system, i.e. the emission duration, and several decades afterwards.

In the toxicity dynamic model, a finer time grid is necessary in order to capture the inventory information and for the resolution of the ODE system. The maximum time step could be set at the lowest LCI time step (e.g. 0.5 days).

Finely, the comparison with conventional LCA results shows that the dynamic toxicity results are very different in many aspects: (i) quantitatively, only the cumulated toxicity could be compared with conventional one; (ii) dynamic approach is more close to the risk assessment methods where the real state of the substance in environment is identified and, from this point of view, the relevance of LCA result is improved; (iii) cumulated toxicity results can be very different from the conventional ones (e.g. 10 times, 100 times), depending on the case study and on the point in time analysed; (iv) the position in time of the toxicity potential can be obtained only with a dynamic approach (e.g. for peoples living after the end of emissions there is no/less toxic potential from organics but still a toxic potential from inorganics).

Acknowledgments

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Appendix A. Supplementary data

A Supplementary Information document is available containing calculation details, data and detailed results. Supplementary data to this article can be found online at doi:https://doi.org/10.1016/j.scitotenv.2017.12.220.

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